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Redox trends in cyclometalated palladium(II) complexes

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Abstract

© The Royal Society of Chemistry.A series of diverse binuclear and mononuclear cyclometalated palladium(ii) complexes of different structure was investigated by electrochemical techniques combined with density functional theory (DFT) calculations. The studies including cyclic and differential pulse voltammetry, X-ray structure analysis and quantum chemical calculations revealed a regularity of the complexes oxidation potential on the metal-metal distance in the complexes: the larger Pd-Pd distance, the higher oxidation potentials. The reduction potentials feature unusually high negative values while no correlation depending on the structure could be observed. These results are in a good agreement with the electron density distribution in the complexes. Additionally, ESR data obtained for the complexes upon oxidation is reported.

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